Package ‘leapgp’

August 1, 2024

Type Package

Title Localized Ensemble of Approximate Gaussian Processes

Version 1.0.0

Author Kellin Rumsey [aut, cre]

Maintainer Kellin Rumsey <knrumsey@lanl.gov>

Description An emulator designed for rapid sequential emulation (e.g., Markov chain Monte Carlo applications). Works via extension of the 'laGP' approach by Gramacy and Apley (2015 <doi:10.1080/10618600.2014.914442>). Details are given in Rumsey et al. (2023 <doi:10.1002/sta4.576>).

License GPL (>= 3)

Encoding UTF-8

RoxygenNote 7.2.3

Imports laGP, RANN, cluster

Suggests knitr, rmarkdown, testthat, lhs, tictoc, RColorBrewer

NeedsCompilation no

Repository CRAN

Date/Publication 2024-08-01 09:30:05 UTC

Contents

leapGP ................................................................. 2
predict_leapGP .................................................. 3

Index 6
leapGP  
Localized Ensemble of Approximate Gaussian Processes

Description

Function to train or initialize a leapGP model, as described in Rumsey et al. (2023).

Usage

leapGP(
  X, 
  y, 
  M0 = ceiling(sqrt(length(y))), 
  rho = NA, 
  scale = FALSE, 
  n = ceiling(sqrt(length(y))), 
  start = NA, 
  verbose = FALSE, 
  justdoit = FALSE,
  ...
)

Arguments

X  
a matrix of training locations (1 row for each training instance)

y  
a vector of training responses (length(y) should equal nrow(X))

M0  
the number of prediction hubs desired. Defaults to ceiling(sqrt(length(Y))).

rho  
(optional). The parameter controlling time-accuracy tradeoff. Can also be specified during prediction.

scale  
logical. Do we want the scale parameter to be returned for predictions? If TRUE, the matrix $K^{-1}$ will be stored for each hub.

n  
local neighborhood size (for laGP)

start  
number of starting points for neighborhood (between 6 and n inclusive)

verbose  
logical. Should status be printed? Default is FALSE

justdoit  
logical. Force leapGP to run using specified parameters (may take a long time and/or cause R to crash).

...  
optional arguments to be passed to laGP()

Details

The leapGP is extends the laGP framework of Gramacy & Apley (2015). The methods are equivalent for rho=1, but leapGP trades memory for speed when rho < 1. The method is described in Rumsey et al. (2023) where they demonstrate that leapGP is faster than laGP for sequential predictions and is also generally more accurate for some settings of rho.
Value

an object of class `leapGP` with fields `X`, `y`, and `hubs`. Also returns scale parameter if `scale=TRUE`.

References


Examples

```r
# Generate data
f <- function(x){
  1.3356*(1.5*(1-x[1]) + exp(2*x[1] - 1)*sin(3*pi*(x[1] - 0.6)^2) +
  exp(3*(x[2]-0.5))*sin(4*pi*(x[2] - 0.9)^2))
}
X <- matrix(runif(200), ncol=2)
y <- apply(X, 1, f)

# Generate data for prediction
Xtest <- matrix(runif(200), ncol=2)
ytest <- apply(Xtest, 1, f)

# Train initial model
mod <- leapGP(X, y, M0 = 30)
# Make sequential predictions
pred <- rep(NA, 100)
for(i in 1:100){
  mod <- predict_leapGP(mod, matrix(Xtest[i,], nrow=1), rho=0.9)
  pred[i] <- mod$mean
}
```

predict_leapGP

**Predict Method for leapGP**

**Description**

Predict method for an object of class `leapGP`. Returns a (possibly modified) `leapGP` object as well as a prediction (with uncertainty, if requested).

**Usage**

```r
predict_leapGP(
  object,
  newdata,  # Optional
  rho = 0.95,  # Default 0.95
  scale = FALSE,  # Optional
)```
predict_leapGP

n = ceiling(sqrt(length(y))),
start = NA,
M_max = Inf,
...
)

Arguments

object
An object of class leapGP

newdata
New data

rho
parameter controlling time-accuracy tradeoff (default is rho=0.95)

scale
logical. Do we want the scale parameter to be returned for predictions? If TRUE, the matrix $K^{-1}$ will be stored for each hub.

n
local neighborhood size

start
number of starting points for neighborhood (between 6 and n inclusive)

M_max
the maximum number of hubs allowed (used to upper bound the run time)

...
optional arguments to be passed to laGP()

Details

The leapGP is extends the laGP framework of Gramacy & Apley (2015). The methods are equivalent for rho=1, but leapGP trades memory for speed when rho < 1. The method is described in Rumsey et al. (2023) where they demonstrate that leapGP is faster than laGP for sequential predictions and is also generally more accurate for some settings of rho.

Value

A list containing values mean, hubs X and y. If scale=TRUE the list also contains field sd.

References


Examples

# Generate data
f <- function(x){
  1.3356*(1.5*(1-x[1]) + exp(2*x[1] - 1)*sin(3*pi*(x[1] - 0.6)^2) +
  exp(3*(x[2]-0.5))*sin(4*pi*(x[2] - 0.9)^2))
}
X <- matrix(runif(200), ncol=2)
y <- apply(X, 1, f)

# Generate data for prediction
Xtest <- matrix(runif(200), ncol=2)
ytest <- apply(Xtest, 1, f)

# Train initial model
mod <- leapGP(X, y, M0 = 30)
# Make sequential predictions
pred <- rep(NA, 100)
for(i in 1:100){
  mod <- predict_leapGP(mod, matrix(Xtest[i,], nrow=1), rho=0.9)
  pred[i] <- mod$mean
}

Index

leapGP, 2

predict_leapGP, 3